



Supplement of

High-resolution air quality simulation over Europe with the chemistry transport model CHIMERE

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The statistical indicators selected for the operational evaluation are defined as follow:

$$OM = \frac{1}{N} \sum_{t=1}^N obs \quad (A1)$$

$$MM = \frac{1}{N} \sum_{t=1}^N mod \quad (A2)$$

$$\sigma_{obs} = \sqrt{\frac{1}{N} \sum_{t=1}^N (obs(x, t) - \overline{obs}(x))^2} \quad (A3)$$

$$\sigma_{mod} = \sqrt{\frac{1}{N} \sum_{t=1}^N (mod(x, t) - \overline{mod}(x))^2} \quad (A4)$$

$$FB = \frac{1}{N} \sum_{t=1}^N \frac{|mod(x, t) - obs(x, t)|}{(obs(x, t) + mod(x, t))/2} \quad (A5)$$

$$FE = \frac{1}{N} \sum_{t=1}^N \frac{|mod(x, t) - obs(x, t)|}{(obs(x, t) + mod(x, t))/2} \quad (A6)$$

$$R = \frac{\sum_{t=1}^N (mod(x, t) - \overline{mod}(x)) \cdot (obs(x, t) - \overline{obs}(x))}{\sqrt{\sum_{t=1}^N (mod(x, t) - \overline{mod}(x))^2} \cdot \sqrt{\sum_{t=1}^N (obs(x, t) - \overline{obs}(x))^2}} \quad (A7)$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{t=1}^N (mod(x, t) - obs(x, t))^2} \quad (A8)$$

$mod(x, t)$ – computed concentration; $obs(x, t)$ – observed concentration; N – number of pairs.

A cut-off threshold has been applied to the observed concentrations to avoid numerical problems due to unrealistic observations. The thresholds have been derived empirically having a look at observed time series. They have been selected in order to preserve as much as possible the original observed data. Thresholds have been defined as follows:

$$NO_2 = 0.5 \text{ ppb}; O_3 = 5 \text{ ppb}; PM_{10} = 1 \mu\text{g m}^{-3}; PM_{2.5} = 1 \mu\text{g m}^{-3}.$$

$$SO_4^{2-} = 0.01 \mu\text{g m}^{-3}; NO_3^- = 0.01 \mu\text{g m}^{-3}; NH_4^+ = 0.01 \mu\text{g m}^{-3}.$$

$$TNO_3^- = 0.01 \mu\text{g m}^{-3}; TNH_4^+ = 0.01 \mu\text{g m}^{-3}.$$

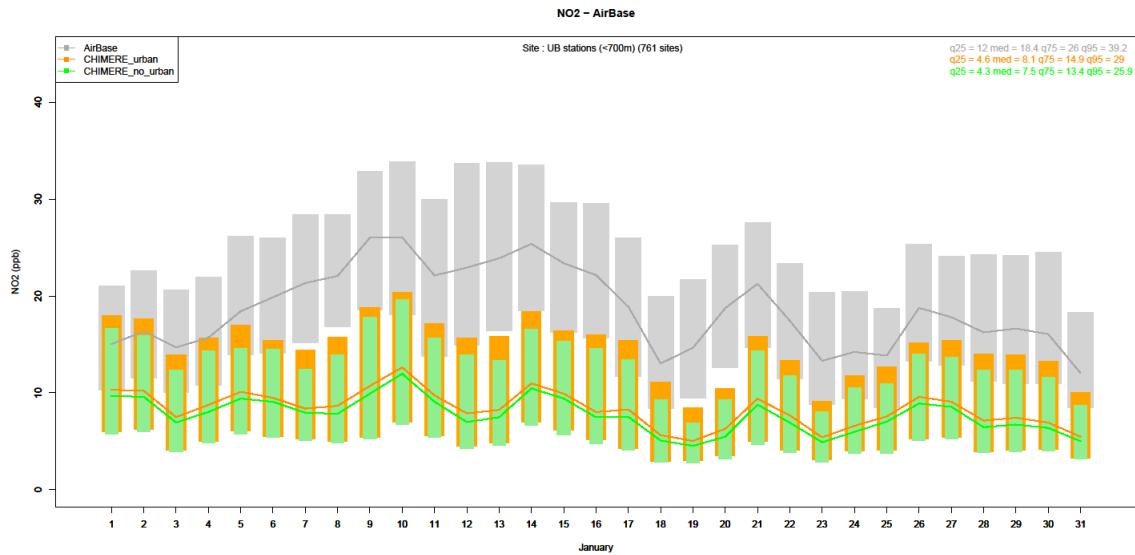


Figure 1s: Daily box-whisker plots time series of the NO₂ observed and calculated (with and without the urban correction) concentrations averaged over all UB AirBase stations for January 2009. The continuous lines represent the medians and the bars show the 25th -75th quantile interval. The yearly 25th (q25), 50th (q50), 75th (q75), and 95th (q95) quantiles are reported on the top right corner of the plots.

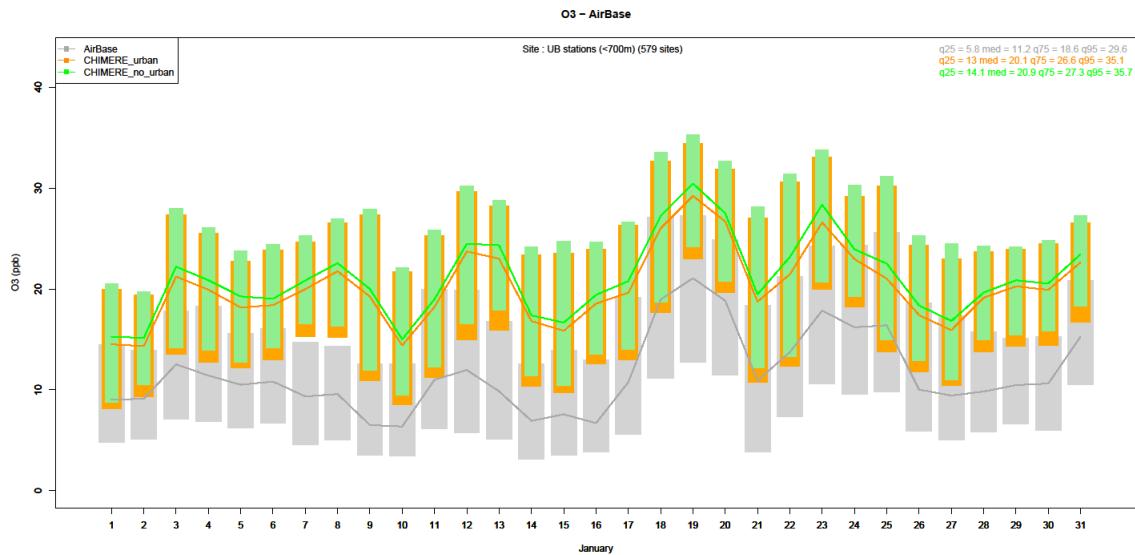


Figure 2s: Same as for Figure 6s but for O₃.

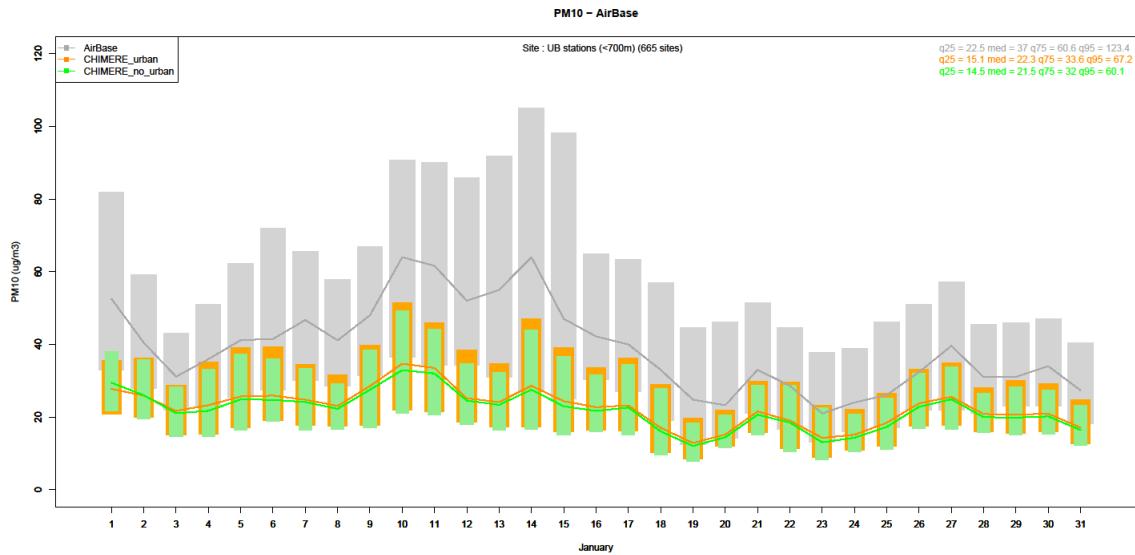


Figure 3s: Same as for Figure 6s but for PM₁₀.

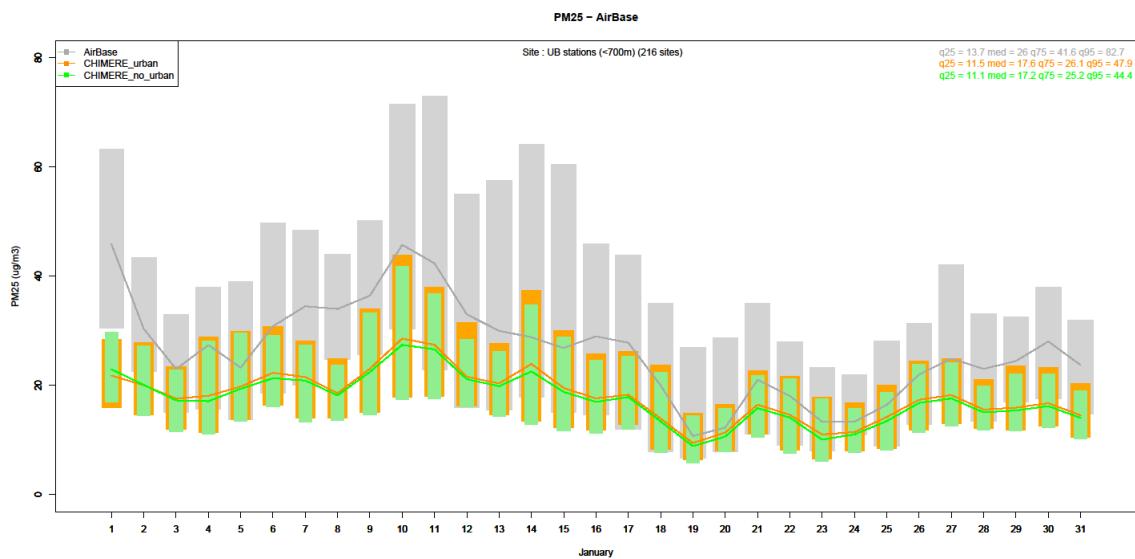


Figure 4s: Same as for Figure 6s but for PM_{2.5}.

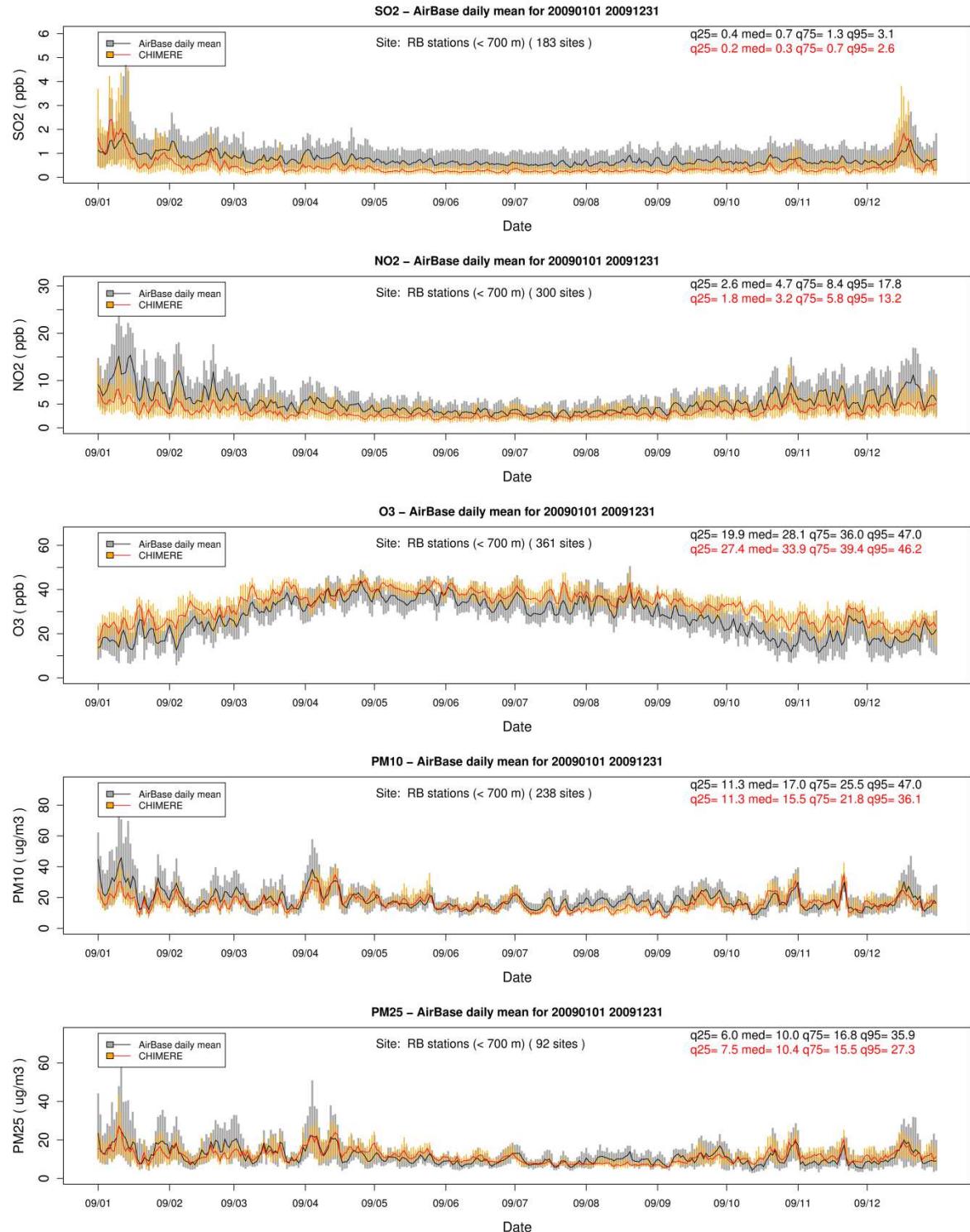


Figure 5s: Daily box-whisker plots time series of the SO₂, NO₂, O₃, PM₁₀ and PM_{2.5} observed and calculated concentrations averaged over all RB AirBase stations. The continuous lines represent the medians and the bars show the 25th -75th quantile interval. The yearly 25th (q25), 50th (q50), 75th (q75), and 95th (q95) quantiles are reported on the top right corner of the plots.

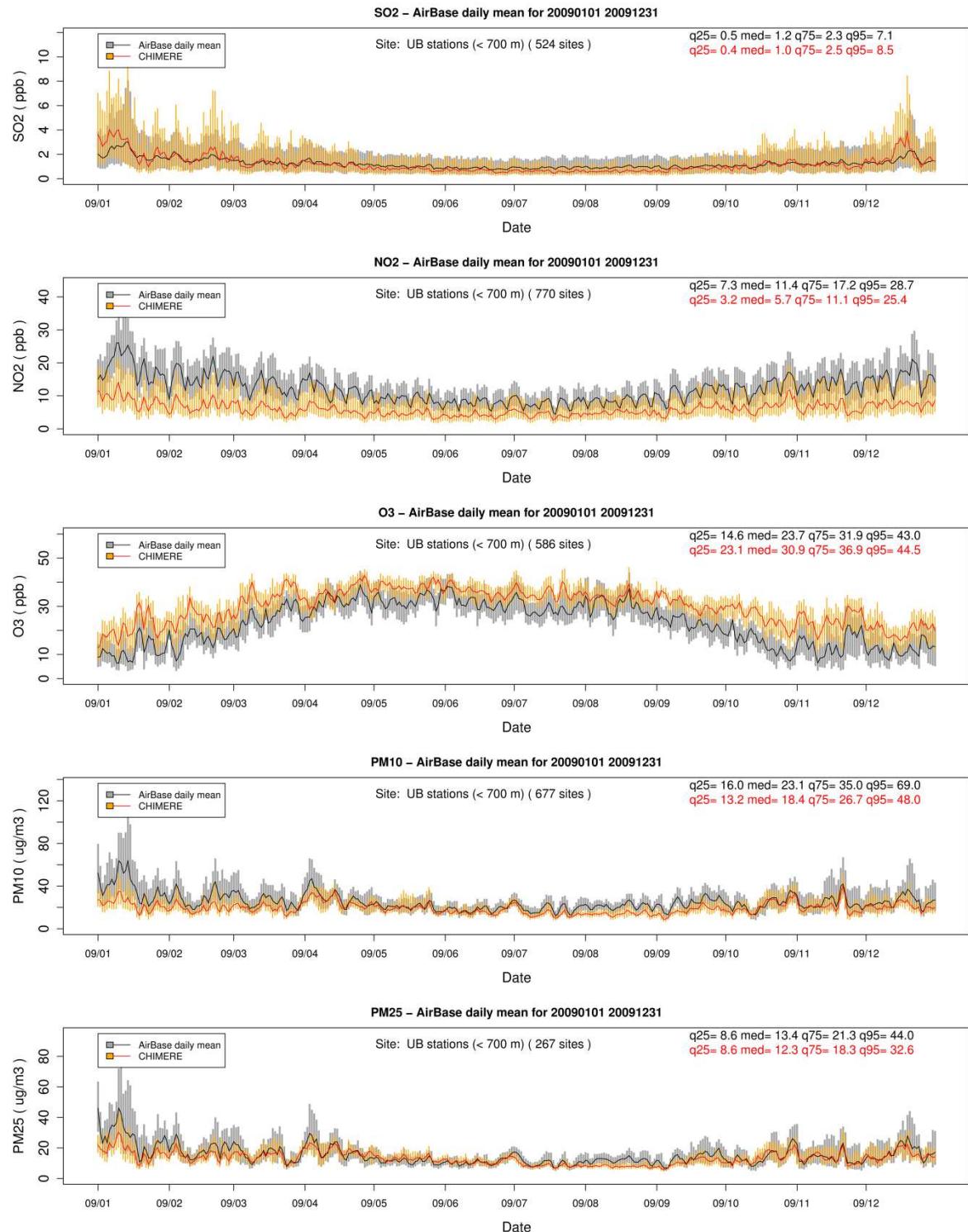


Figure 6s: Same as Figure 1s but averaged over all UB AirBase stations.

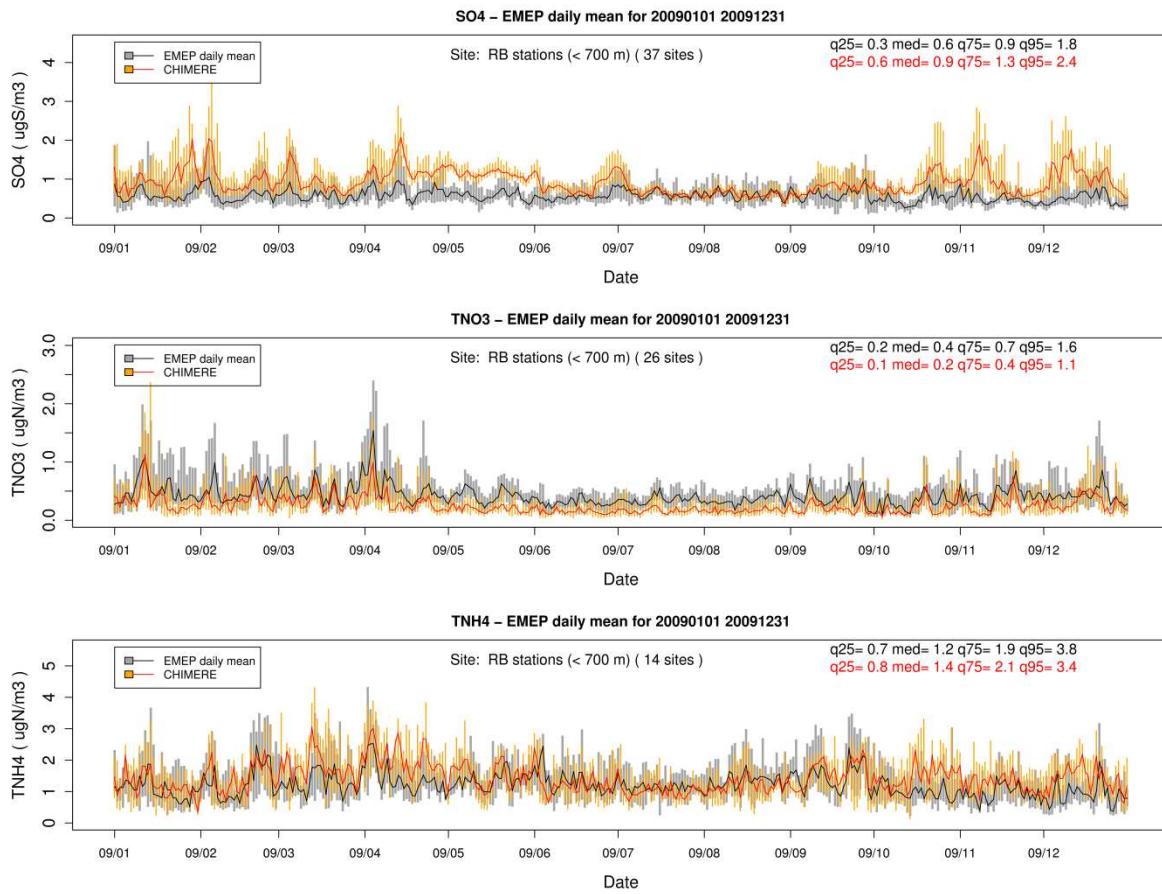


Figure 7s: Same as Figure 2s but for sulphate, total nitrate ($\text{HNO}_3+\text{NO}_3^-$) and total ammonia ($\text{NH}_3+\text{NH}_4^+$) averaged over all RB EMEP stations

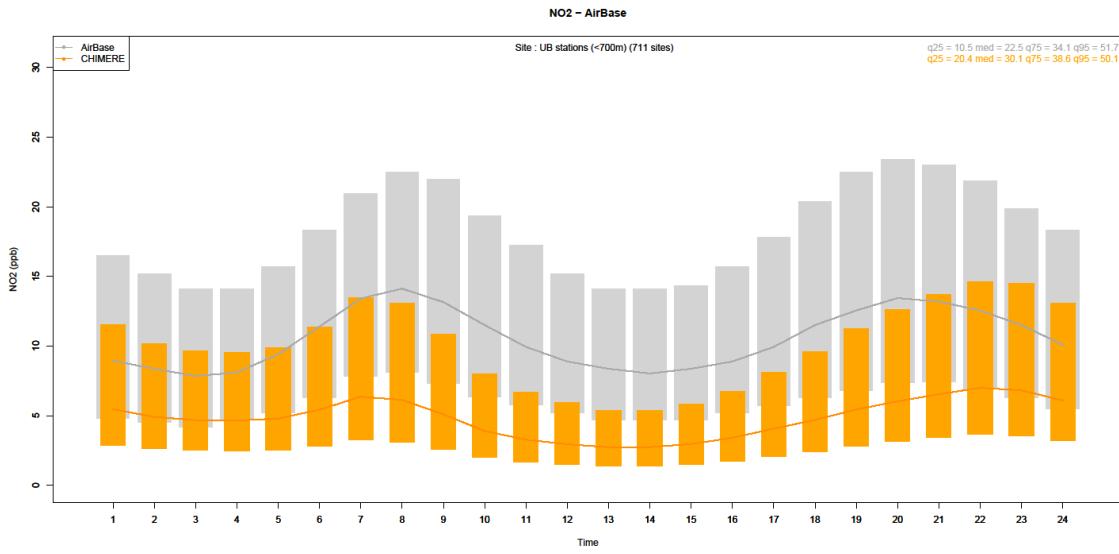


Figure 8s: Annual mean daily cycle box-whisker plots time series for the NO_2 observed and calculated concentrations averaged over all UB AirBase stations. The continuous lines represent the medians and the bars show the 25th -75th quantile interval. The yearly 25th (q_{25}), 50th (q_{50}), 75th (q_{75}), and 95th (q_{95}) quantiles are reported on the top right corner of the plots.

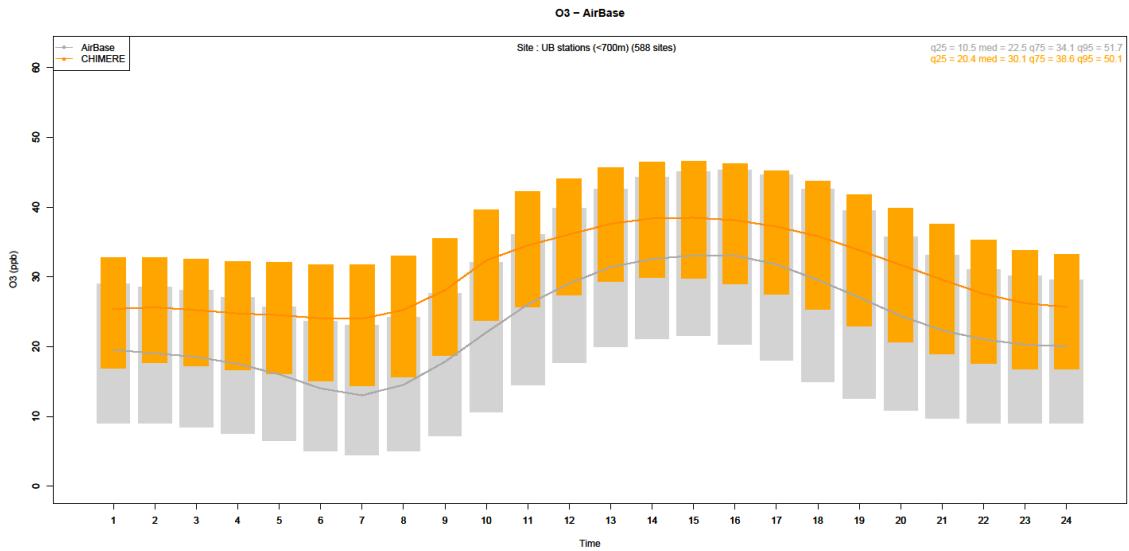


Figure 9s: Same as figure 4s but for the O_3 .